

Isopropyl carbamate
1746-77-6 | DTXSID9051795

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 4.67e-01

Global applicability domain: Inside

Local applicability domain index: 6.69e-01

Confidence level: 7.53e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Propyl carbamate</div> <div>Measured: 0.36</div> <div>Predicted: 3.70e-01</div>	<div>Image not found</div> <div>Carbamic acid, butyl ester</div> <div>Measured: 0.85</div> <div>Predicted: 8.43e-01</div>	<div>Image not found</div> <div>Carbamic acid, 2-methylpropyl ester</div> <div>Measured: 0.65</div> <div>Predicted: 7.83e-01</div>
<div>Image not found</div> <div>Urethane</div> <div>Measured: -0.150</div> <div>Predicted: -0.120</div>	<div>Image not found</div> <div>tert-Butyl carbamate</div> <div>Measured: 0.48</div> <div>Predicted: 7.13e-01</div>	